November 2, 2001

Reporting Requirements

Workshop participants agreed on slight modifications to some of the problem specifications, and determined specific reporting requirements. Results for different problems should be submitted to the respective coordinators (see below). Also, contact coordinators if you need any clarifications of problem specifications and reporting requirements.

Results should be submitted as tabular data, to facilitate plotting of results from different groups. Figures should also be submitted, to minimize the possibility that tabular data may be misread by the coordinators. SI units should be used throughout (kg, s, m^3, Pa, ˚C). Concentrations can be given either as mole fractions or mass fractions, depending on the problem specifications.

When using mole fractions, please specify whether moles of Na and Cl are counted separately or not. (A 1-molar solution of NaCl has 1 mole of Na and 1 mole of Cl; different conventions are possible depending upon whether or not this is counted as 2 moles of solutes. Please specify what you're using. This potential ambiguity in the convention for counting moles is one reason I prefer mass fractions!)

I use the terms "liquid" and "aqueous" phase interchangeably. The CO_2-rich phase I denote for simplicity as "gas," even if from a strict thermodynamics viewpoint this may be a supercritical phase, and one could argue about whether or not this is "liquid" or "gas." - I count a year as 365.25 days (including 1/4 of a leap day), or 31.5576×10^6 seconds.

The deadline for submitting final results is February 28th, 2002. Participants are encouraged to submit their results earlier, to allow some time for clarification or resolution of any issues that may come up.

Problem # 1 - "stratified gas"
(coordinator Curt Oldenburg, LBNL; e-mail CMOldenburg@lbl.gov)

The problem should be started from initial conditions of uniform pressure. Two variations should be run, P = 40 bar and 100 bar. No further variations are desired.

Give vertical profiles of pressure, density, viscosity, and mole fractions in gas at times t = 0, 10 yr, 50 yr, and 100 yr.

Give fluid property data at P = 40 bar and 100 bar, for CO_2 mole fractions of 0, 0.5, and 1. The data should include density, viscosity, and mole fractions of both gases in water.

Problem # 2 - "lateral gas"
(coordinator Curt Oldenburg, LBNL; e-mail CMOldenburg@lbl.gov)

The problem should be started from initial conditions of uniform pressure. Two variations should be run, P = 40 bar and 100 bar. No further variations are desired.

Give vertical profiles at x = 25 m and 75 m, and a horizontal profile at z = 50 m, at times t = 0.5 yr, 1 yr, 2 yr, 5 yr, and 10 yr. Data along the profiles should include pressure, density, viscosity, and mole fractions in gas.

Give fluid property data at P = 40 bar and 100 bar, for CO_2 mole fractions of 0, 0.5, and 1. The data should include density, viscosity, and mole fractions of both gases in water.

Problem # 3 - "radial aquifer"
(coordinator Karsten Pruess, LBNL; e-mail K_Pruess@lbl.gov)

The problem specifications will be used as given (no changes). Variations will be limited to two cases, namely, with and without salinity. Results are to be given for pressure, gas saturation, dissolved CO_2 mass (or mole) fraction, and "solid saturation" (fraction of pore volume containing solid precipitate). The problem as posed is known to have a similarity solution, with all parameters depending on radial distance R and time t only through the similarity variable $\xi = R^2/t$. Results can be given either as radial profiles at a fixed time, or as time series at a fixed radial distance. It is preferred that both kinds of results should be submitted, to allow checking on the similarity property. It is desired that results should be provided for such a range of times and distances that the similarity variable covers the range 10^{-8} m^2/s $\le \xi \le 10^{1}$ m^2/s.

In addition, fluid property data should be given at T = 45 ˚C for pressures P = 120, 160, 200, and 240 bar, for aqueous phase salinities of 0 and 15 weight-%, and for phase conditions of (a) single-phase aqueous, (b) two-phase aqueous-gas. The fluid property data should include densities and viscosities of aqueous and gas phases, and CO_2 mass (or mole) fractions in the aqueous phase.

Problem # 4 - "fault discharge"
(coordinator Karsten Pruess, LBNL; e-mail K_Pruess@lbl.gov)

The problem specifications will be used as given (no changes). No variations will be pursued. Give results for mass fluxes of CO_2 (kg/m^2 s), summed over liquid and gas phases, at inlet (bottom) and outlet (top). Also give aqueous phase flux at the outlet. Fluxes should be reported for a range of times 10^3 s $\le$ t $\le 10^{11}$ s. Also provide profiles of gas saturation and CO_2 mass (or mole) fraction at times of 10^7 and $2x10^7$ s. Report CO_2 inventory at times of 10^7 and $2x10^7$ s, separately for aqueous and gas phases.

Give fluid property data for the same conditions as specified in problem # 3, except in problem # 4 there is no salinity.

Problem # 5 - "mineral trapping"
(coordinator Tianfu Xu, LBNL; e-mail Tianfu_Xu@lbl.gov)

Two variations should be run, (1) as originally specified (and using thermodynamic data for glauconite as separately provided by Tianfu), (2) using annite instead of glauconite, and removing the organic matter and redox reactions (replace the 2.64 volume-% organic with quartz).

Results should be given as originally specified for times up to 10^5 yr. Aqueous concentrations should be reported in units of moles per kg H_2O. Amounts of CO_2 sequestered should be given as kg per m^3 of medium.

Problem # 6 - "hydromechanical"
(coordinator Jonny Rutqvist, LBNL; e-mail JRutqvist@lbl.gov)

The problem specifications will be used as given. A variation was added that involves neglecting mechanical changes; it is hoped that this will encourage participation from people who do not have a capability for coupled mechanical processes.

Definition of results to be calculated is as given in the original problem description, with the following two modifications, (a) add reporting at a time of t = 10 yr, and (b) do not report CO_2 flux at the ground surface.

Fluid property data should be given for mixtures of pure water and CO_2 at conditions of (T, P) = (30 MPa, 55 ˚C), (23 MPa, 49 ˚C), and (12 MPa, 46 ˚C). The data should include density and viscosity of liquid and gas phases, mass (or mole) fractions of CO_2 in the aqueous phase, and mass (or mole) fractions of water in the gas phase.

Problem # 7 - "layered brine"

(coordinator Carl Steefel, LLNL; e-mail steefel1@llnl.gov)

There is one change in problem specifications: for gas relative permeability, a Corey function should be used as formulated for problem # 3, with parameters of $S_{lr} = 0.2$, $S_{gr} = 0.05$. The problem should be run in two variations, with and without salinity. Injection should be made uniformly over a region of 1x1x1 m^3, that extends from 0 m ≤ x ≤ 1 m, and 21.5 m ≤ z ≤ 22.5 m.

Give results for pressure, gas saturation, CO_2 mass (or mole) fraction in the aqueous phase, and water mass (or mole) fraction in the gas phase. These data should be given as vertical profiles at x = 10 m, 200 m, 500 m, and 1000 m, and as horizontal profiles at the centers of the second and third sands (counted from the bottom; this corresponds to elevations of 70 m and 103 m, respectively, from the bottom). The profiles should be given at times of 1 month (= 30 days), 1 yr, and 2 yr.

In addition provide data for total mass of CO_2 versus time, separately for each of the five sands. Also give the fraction of CO_2 in the system in the aqueous phase versus time. Time runs out to two years. To facilitate analysis, give contour plots of gas saturation at times of 1 yr and 2 yr.

Give fluid property data at T = 37 ˚C, P = 90, 100, 120, 140, 160, 180 bar, for (a) pure water, (b) 3.2 weight-% salinity, (c) NaCl-saturated brine. The data should include density and viscosity of aqueous and gas phases, mass (or mole) fraction of CO_2 in the aqueous phase, and mass (or mole) fraction of water in the gas phase. Report data for single-phase aqueous conditions with a CO_2 partial pressure of $PCO_2 = 0.5$ bar, as well as for two-phase conditions. Also give NaCl weight-% in saturated brine.

Problem # 8 - "CO_2-oil"

(coordinator Tony Kovscek, Stanford U.; e-mail kovscek@pangea.Stanford.EDU)

As additional specification an absolute permeability of 10^{-12} m^2 (1 darcy) should be used. Participants should use their own fluid property descriptions, and should report data defining the two-phase envelope in T-P space. Care should be taken to use "sufficiently" fine gridding.

Report gas saturations and mole fractions of all components versus the similarity variable x/t.